Cyclobutanecarboxylic acid, 1-((4-chlorophenyl)sulfonyl)-, 1-methylethyl ester
160790-09-0 | DTXSID20166995

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 331 °C

Global applicability domain: Inside

Local applicability domain index: 3.35e-01

Confidence level: 4.89e-01

Nearest Neighbors from the Training Set

Image not found
Benzene, 1,1'-sulfonylbis[4-methyl-
Measured: 406
Predicted: 360

Image not found
Diphenylsulfone
Measured: 279
Predicted: 315

Image not found
1,3-Benzodioxole, 4,7-dimethoxy-5-(2-propenyl)-
Measured: 294
Predicted: 287

Image not found
Chlorthal-dimethyl
Measured: 365
Predicted: 345